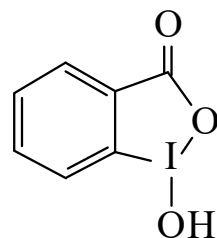




>>Entry Name: 1-Hydroxy-1,2-benziodoxol-3(1*H*)-one, 9Cl, 8Cl

Synonym(s): 1,3-Dihydro-1-hydroxy-3-oxo-1,2-benziodoxole. 3-Oxo-3*H*-1,2-benziodoxol-1-ium hydroxide



CAS Registry Number: 131-62-4

Molecular Formula: C₇H₅IO₃

Molecular Weight: 264.019

Accurate Mass: 263.928343

Percentage Composition: C 31.85%; H 1.91%; I 48.07%; O 18.18%

Use/Importance: Enzyme inhibitor. Reagent for determination of xanthates. Catalyst for cleavage of reactive phosphates in cationic surfactant soln.

Physical Description: Cryst. (H₂O)

Melting Point: Mp 231-232 dec.°

pKa Value: p*K*_a 6.22

Hazard & Toxicity: LD₅₀ (mus, ipr) 175 mg/kg

>>Derivative: Ac

Molecular Formula: C₉H₇IO₄

Molecular Weight: 306.056

Accurate Mass: 305.938908

Percentage Composition: C 35.32%; H 2.31%; I 41.46%; O 20.91%

Physical Description: Cryst. (Ac₂O)

Melting Point: Mp 167-169°

>>Derivative: Me ether

Synonym(s): 1-Methoxy-1,2-benziodoxol-3(1*H*)-one

Molecular Formula: C₈H₇IO₃

Molecular Weight: 278.046

Accurate Mass: 277.943993

Percentage Composition: C 34.56%; H 2.54%; I 45.64%; O 17.26%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 166-168 and ca. 190°° (double Mp)

>>Derivative: 1-Oxide

CAS Registry Number: 61717-82-6

Molecular Formula: C₇H₅IO₄

Molecular Weight: 280.019

Accurate Mass: 279.923258

Percentage Composition: C 30.03%; H 1.80%; I 45.32%; O 22.85%

Physical Description: Solid

Melting Point: Mp 232-233 dec.°

Solubility: Insol. common org. solvs.

Hazard & Toxicity: Explosive

>>Derivative: *O*-Methanesulfonyl

Molecular Formula: C₈H₇IO₅S

Molecular Weight: 342.111

Accurate Mass: 341.905893

Percentage Composition: C 28.09%; H 2.06%; I 37.09%; O 23.38%; S 9.37%

Physical Description: Cryst.

Melting Point: Mp 174-176°

Other Data: Hygroscopic, forms pentahydrate in air